

The finite-temperature thermodynamics of a trapped unitary Fermi gas within fractional exclusion statistics

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We utilize a fractional exclusion statistics of Haldane and Wu hypothesis to study the thermodynamics of a unitary Fermi gas trapped in a harmonic oscillator potential at ultra-low finite temperature. The entropy per particle as a function of the energy per particle and energy per particle versus rescaled temperature are numerically compared with the experimental data. The study shows that, except the chemical potential behavior, there exists a reasonable consistency between the experimental measurement and theoretical attempt for the entropy and energy per particle. In the fractional exclusion statistics formalism, the behavior of the isochore heat capacity for a trapped unitary Fermi gas is also analyzed.

Keywords: Trapped fermion thermodynamics; unitary Fermi gas; fractional exclusion statistics

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I. INTRODUCTION

The thermodynamics of a strongly interacting fermion system attracts much attention, either experimentally or theoretically, in the many-body community in recent years [1]. For the dilute contact interacting atomic system, the scattering length a describes the mutual interaction strength between two fermions. With the Feshbach resonance technology, it is possible to tune the s -wave scattering length a through changing the external magnetic field. The scattering length a can be changed from a negative value to the other side of the resonance where a becomes positive. In the weak attraction Bardeen-Cooper-Schrieffer (BCS) regime with $k_F|a| \ll 1$ (with the Fermi wave vector k_F), the mean field theory can give a reasonable description. With the increase of the interaction strength, the composite bosons can be formed in the fermion system, where the Bose-Einstein condensation (BEC) can occur [1, 2].

In the regime from negative scattering length to positive value, the two-body interaction strength can be singular with the existence of a zero-energy bound state. The limit $k_F|a| \rightarrow \infty$ is called BCS-BEC crossover, which is also called the unitary regime [1]. The corresponding gas in this limit is called unitary Fermi gas [2]. At unitarity, the gas both has some properties of fermions and some of bosons, that is to say, the behavior of this gas is between that of fermions and bosons. The fermion system will show a universal thermodynamic behavior near the resonance point where the scattering length a diverges [1, 2].

Initially, physicists concentrated on the energy density per particle of the unitary Fermi gas at zero temperature theoretically. For a homogeneous gas, the ground-state

energy per particle is given by $E/N = \frac{3}{5}\xi E_F$ with the ideal Fermi energy E_F and the universal coefficient ξ [2]. It is $E/N = \frac{3}{4}\sqrt{\xi}E_F$ for a trapped unitary gas, where E_F is the Fermi energy of the trapped noninteracting Fermi gas [3]. Determining the dimensionless constant ξ has been an important physical subject in the past few years.

Furthermore, exploring the thermodynamics of a unitary Fermi gas at finite temperature in theory to explain the experimental results is a more challenging task. A diagrammatic determinant Monte Carlo method for the negative- U Hubbard model was used to calculate the finite-temperature thermodynamics of a homogeneous unitary gas [4]. Through the quantum Monte Carlo simulation, the finite-temperature thermodynamics of a homogeneous unitary gas can be given by Refs.[5, 6]. A self-consistent theory based on the combined Luttinger-Ward-De Dominicis-Martin variational formalism was also used to calculate it for a homogeneous unitary gas [7].

For the finite-temperature thermodynamics of a trapped unitary Fermi gas, the entropy and energy of the trapped unitary Fermi system have been experimentally measured in Refs.[8–10]. The quantum Monte Carlo simulation can also be used to calculate the finite-temperature thermodynamics of a trapped unitary gas [11]. Various theoretical attempts have been established to give the calculations for a trapped unitary Fermi gas. The pseudogap theory is one of them [12, 13]. A mean-field method by solving the Bogoliubov-de Gennes equations with an efficient and accurate method was used in Ref.[14]. A T -matrix calculation with a modified Nozières and Schmitt-Rink approximation was adopted to explore it [15]. The combined Luttinger-Ward-De Dominicis-Martin variational formalism was also proved to be a valuable approach for it [16]. We note that there are still differences among in these attempts on the finite-temperature thermodynamic properties of a unitary Fermi gas.

Due to the scale invariance at unitarity, the thermo-

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dynamic properties of the universal strongly interacting unitary fermions are related to those of the non-interacting ideal fermions. This means that the dynamical details will not appear in the final thermodynamic analytical expressions. From the microscopic point of view, the unitary fermions system is in between the fermionic and composite bosonic phases. To characterize this crossover or intermediate unitary fermionic thermodynamics, Haldane-Wu fractional exclusion statistics was used to discuss the finite-temperature unitary Fermi gas thermodynamics [17, 18]. In physics, the thermodynamic behavior of the fractional exclusion statistics is between those of Bose-Einstein and Fermi-Dirac statistics [19, 20], which is quite similar to the thermodynamics of real fermions at unitarity. As a hypothesis, the strongly interacting unitary gas is modeled by the non-interacting anyons. The priority is that the finite-temperature thermodynamic properties can be investigated analytically [21]. The quintessence hidden in this attempt is that the anyonic statistical parameter g characterizes the strongly interacting universal properties.

Following the fractional exclusion statistics formalism, the aim of this work is to give a detailed discussion on the trapped gas thermodynamics. By generalizing the discussion for the homogeneous unitary system [22], we want to give the expressions and the corresponding numerical results of entropy, physical chemical potential and isochore heat capacity of a trapped unitary system. The concrete comparisons with experimental measurements are made.

The natural units $k_B = \hbar = 1$ are used throughout the paper.

II. FINITE-TEMPERATURE THERMODYNAMICS WITHIN FRACTIONAL EXCLUSION STATISTICS

A. Framework of fractional exclusion statistics

In this subsection, we will briefly review the formalism of the fractional exclusion statistics. By generalizing the simple formula with the fractional exclusion statistics, one can get the microscopic quantum states W of N identical particles occupying a group of G states [20, 22]

$$W = \prod_i \frac{[G_i + (N_i - 1)(1 - g)]!}{N_i! [G_i - gN_i - (1 - g)]!}, \quad (1)$$

where g is a statistical parameter, which denotes the number of states that one particle can occupy. For bosons, $g = 0$ and $g = 1$ for fermions.

If G_i and N_i are very large, one has the approximate expression of the logarithm of W

$$\begin{aligned} \ln W &\simeq \sum_i [(G_i + (1 - g)N_i) \ln (G_i + (1 - g)N_i) \\ &\quad - (G_i - gN_i) \ln (G_i - gN_i) - N_i \ln N_i], \quad (2) \end{aligned}$$

through the Stirling formula $\ln N! = N(\ln N - 1)$.

The variational formulation of $\ln W$ is

$$\begin{aligned} \delta \ln W &= \sum_i [(1 - g) \ln (G_i + (1 - g)N_i) \\ &\quad + g \ln (G_i - gN_i) - \ln N_i] \delta N_i. \quad (3) \end{aligned}$$

However, δN_i is not arbitrary, it must satisfy the conditions below:

$$\begin{aligned} \delta N &= \sum_i \delta N_i = 0, \\ \delta E &= \sum_i \epsilon_i \delta N_i = 0. \quad (4) \end{aligned}$$

Setting the two Lagrange multipliers $\alpha = -\mu/T$ and $\beta = 1/T$, one can have

$$\begin{aligned} &\delta \ln W - \alpha \delta N - \beta \delta E \\ &= \sum_i [(1 - g) \ln (G_i + (1 - g)N_i) \\ &\quad + g \ln (G_i - gN_i) - \ln N_i + (\mu - \epsilon_i)/T] \delta N_i \\ &= \sum_i \left[(1 - g) \ln \left(1 + \frac{G_i}{N_i} - g \right) \right. \\ &\quad \left. + g \ln \left(\frac{G_i}{N_i} - g \right) + \left(\frac{\mu - \epsilon_i}{T} \right) \right] \delta N_i, \quad (5) \end{aligned}$$

where μ is the chemical potential, T is the system temperature and ϵ_i is the single-particle energy for the state of species i .

Defining the average occupation number $\bar{N}_i \equiv N_i/G_i$, through the Lagrange multiplier method $\delta \ln W - \alpha \delta N - \beta \delta E = 0$, the most probable distribution of \bar{N}_i can be derived from Eq.(5)

$$\bar{N}_i = \frac{1}{\omega_i + g}, \quad (6)$$

where ω_i obeys the relation

$$\mu - \epsilon_i = -T [(1 - g) \ln (1 + \omega_i) + g \ln \omega_i]. \quad (7)$$

In Eq.(7), we define ω_0 as the value of ω_i at $\epsilon_i = 0$. Consequently, one has

$$\mu = -T [(1 - g) \ln (1 + \omega_0) + g \ln \omega_0]. \quad (8)$$

At zero temperature, there is

$$\begin{aligned} \bar{N}_i &= 0, \quad \text{for } \epsilon_i > \mu; \\ \bar{N}_i &= \frac{1}{g}, \quad \text{for } \epsilon_i < \mu. \quad (9) \end{aligned}$$

Furthermore, by inserting Eq.(6) into Eq.(2), one obtains the expression for entropy as

$$S = \ln W = \sum_i \frac{G_i}{\omega_i + g} [(\omega_i + 1) \ln (\omega_i + 1) - \omega_i \ln \omega_i] \quad (10)$$

B. Thermodynamics of a trapped unitary Fermi gas

The finite-temperature thermodynamics can be derived for the unitary Fermi gas trapped in a harmonic oscillator $m\varpi^2 r^2/2$, where the oscillator parameter ϖ is defined as $\varpi = (\omega_x \omega_y \omega_z)^{1/3}$ and r denotes the position of particles. The corresponding density of states is $D(\epsilon) = \epsilon^2/\varpi^3$. At zero temperature, the particle number and system energy are

$$N = \frac{1}{g} \int_0^{\tilde{E}_F} D(\epsilon) d\epsilon = \frac{E_F^3}{3\varpi^3}, \quad (11)$$

$$E = \frac{1}{g} \int_0^{\tilde{E}_F} \epsilon D(\epsilon) d\epsilon = \frac{g^{1/3} E_F^4}{4\varpi^3}, \quad (12)$$

where \tilde{E}_F obeys the relation $\tilde{E}_F = g^{1/3} E_F$ with the ideal Fermi energy $E_F = (3N)^{1/3} \varpi$ in a harmonic oscillator.

Comparing Eq.(11) with Eq.(12) to eliminate ϖ , it is shown that

$$\frac{E}{NE_F} = \frac{3}{4} g^{1/3}. \quad (13)$$

If the statistical parameter g in the fractional exclusion statistics is fixed through the zero-temperature ground-state energy, the finite-temperature thermodynamic quantities for a trapped unitary Fermi gas can be calculated. For the trapped system, the ground-state energy is related with the universal coefficient according to $E/(3/4 NE_F) = \sqrt{\xi}$ [3]. From Eq.(13), it is found that $E/(3/4 NE_F) = g^{1/3}$. So the statistical parameter could be calculated as $g = \xi^{3/2} = \frac{8}{27}$, with $\xi = \frac{4}{9}$ given by the developed quasi-linear approximation method [23–28].

For the finite-temperature trapped unitary Fermi system, the particle number and energy can be represented by turning the sum of quantum state into integral and changing the variable from $d\epsilon$ to $d\omega$

$$N = \sum_i G_i \bar{N}_i = \int_0^\infty \frac{D(\epsilon) d\epsilon}{\omega + g} = \left(\frac{T}{\varpi}\right)^3 h_2(\omega_0), \quad (14)$$

$$E = \sum_i G_i \bar{N}_i \epsilon_i = \int_0^\infty \frac{\epsilon D(\epsilon) d\epsilon}{\omega + g} = \left(\frac{T}{\varpi}\right)^3 T h_3(\omega_0), \quad (15)$$

where

$$h_n(\omega_0) = \int_{\omega_0}^\infty \frac{d\omega}{\omega(1+\omega)} \left[\ln \left(\frac{\omega}{\omega_0} \right)^g \left(\frac{1+\omega}{1+\omega_0} \right)^{1-g} \right]^n.$$

By replacing Eq.(11) into Eq.(14) and Eq.(15), one gets

$$3 \left(\frac{T}{T_F} \right)^3 h_2(\omega_0) = 1, \quad (16)$$

$$\frac{E}{NE_F} = 3 \left(\frac{T}{T_F} \right)^4 h_3(\omega_0), \quad (17)$$

with the Fermi characteristic temperature T_F .

One can turn the sum of Eq.(10) to an integral. With Eq.(16), one can get the explicit integral expression of entropy per particle

$$\begin{aligned} \frac{S}{N} &= 3 \left(\frac{T}{T_F} \right)^3 \int_{\omega_0}^\infty \left[\left(\frac{\ln(\omega+1)}{\omega} - \frac{\ln \omega}{\omega+1} \right) \right. \\ &\quad \left. \times \left(\ln \left(\frac{\omega}{\omega_0} \right)^g \left(\frac{1+\omega}{1+\omega_0} \right)^{1-g} \right)^2 \right] d\omega. \end{aligned} \quad (18)$$

In order to derivate the expression of the isochore heat capacity, let us further discuss the particle number. From Eq.(14), the partial derivative of the particle number N to temperature T for fixed N and ϖ is given by

$$\begin{aligned} \left(\frac{\partial N}{\partial T} \right)_{N, \varpi} &= \frac{3T^2}{\varpi^3} h_2(\omega_0) + \left(\frac{T}{\varpi} \right)^3 \left[\left(\frac{\partial h_2}{\partial T} \right)_\mu \right. \\ &\quad \left. + \left(\frac{\partial h_2}{\partial \mu} \right)_T \left(\frac{\partial \mu}{\partial T} \right)_{N, \varpi} \right]. \end{aligned} \quad (19)$$

From Eq.(19), one can get

$$\left(\frac{\partial \mu}{\partial T} \right)_{N, \varpi} = \frac{\mu}{T} - \frac{3h_2(\omega_0)}{2h_1(\omega_0)}. \quad (20)$$

Furthermore, with Eq.(15) and the thermodynamic relation between the isochore heat capacity C_V and internal energy E , one has

$$\begin{aligned} C_V &= \left(\frac{\partial E}{\partial T} \right)_{N, \varpi} \\ &= 4 \left(\frac{T}{\varpi} \right)^3 h_3(\omega_0) + \left(\frac{T}{\varpi} \right)^3 T \left[\left(\frac{\partial h_3}{\partial T} \right)_\mu \right. \\ &\quad \left. + \left(\frac{\partial h_3}{\partial \mu} \right)_T \left(\frac{\partial \mu}{\partial T} \right)_{N, \varpi} \right]. \end{aligned} \quad (21)$$

Substituting Eq.(14) and Eq.(20) into Eq.(21), one obtains the isochore heat capacity per particle

$$\frac{C_V}{N} = \frac{4h_3(\omega_0)}{h_2(\omega_0)} - \frac{9h_2(\omega_0)}{2h_1(\omega_0)}. \quad (22)$$

III. DISCUSSIONS

Based on the above analytical expressions, we will give the numerical results.

The energy per particle versus the rescaled temperature can be calculated from Eq.(16) and Eq.(17). As indicated by the Fig.1, the energy for the trapped unitary Fermi gas with the statistical parameter $g = \frac{8}{27}$ versus the rescaled temperature is consistent with the experimental data [8].

Through Eq.(17) and Eq.(18), the relation between the entropy per particle and the energy per particle is given

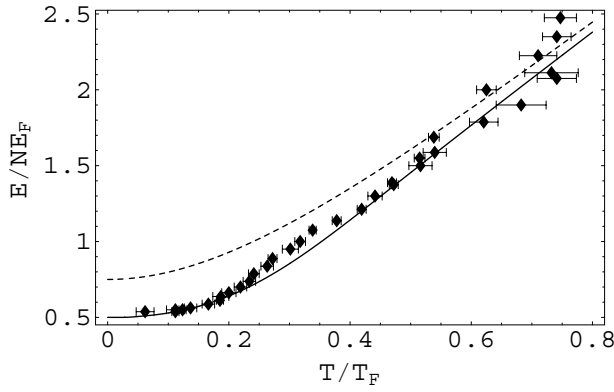


FIG. 1: The energy per particle versus the rescaled temperature. The solid curve denotes that for the trapped unitary Fermi gas, and the dashed one is that for the trapped ideal Fermi gas. The dots with error bars are the experimental data of Refs.[8].

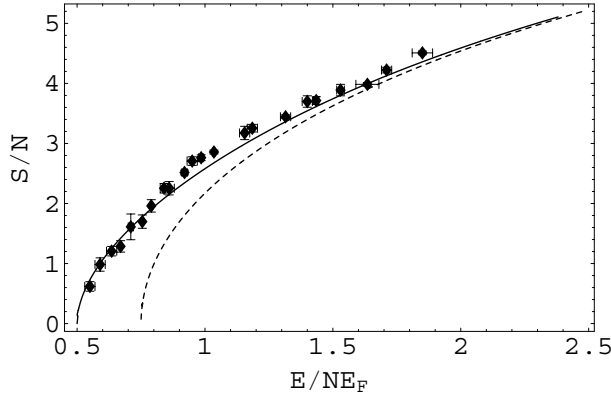


FIG. 2: The entropy per particle plotted as a function of the rescaled energy per particle. The line styles are similar to Fig.1. The dots with error bars are the experimental data of Refs.[9, 10].

explicitly in Fig.2. The entropy increases with increasing energy, and in the Boltzmann regime, the curve for a trapped unitary Fermi gas gets closer to and almost overlaps with that of the trapped ideal Fermi gas. It is found that the theoretical result is reasonably consistent with that of the experiment.

The agreements in Fig.1 and Fig.2 between the theoretical curves and the experimental data show that the statistical parameter g can be capable of describing the strong interaction of unitary Fermi gas at extremely low temperature.

With Eqs.(8), (16) and (17), we have also shown the plot of the chemical potential varying with the rescaled energy per particle in Fig.3. It is a monotonically decreasing function of the energy per particle. In the Boltzmann regime, the curve for a trapped unitary Fermi gas gets closer to that of the trapped ideal one. In the extremely low-temperature regime ($E/(NE_F) < 1.2$), the departure between the theoretical result and the exper-

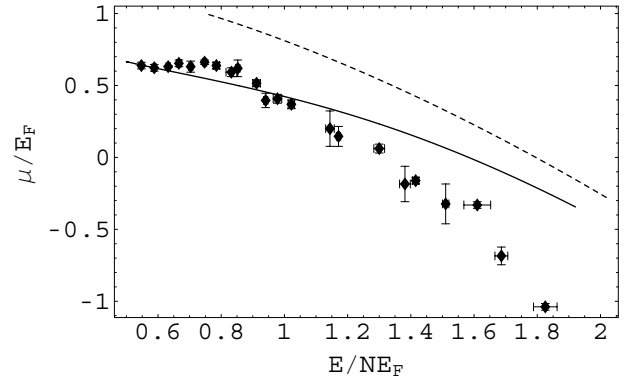


FIG. 3: Similar to Fig.1 for the variation of the chemical potential as a function of the rescaled energy per particle. The dots with error bars are the experimental data of Ref.[10].

imental data is not obvious. However, the chemical potential differs explicitly from the experimental result for $E/(NE_F) > 1.2$. As the temperature increases, the experimental data also diverge from the curve of the trapped ideal gas. We can also plot the chemical potential versus the rescaled temperature in Fig.4.

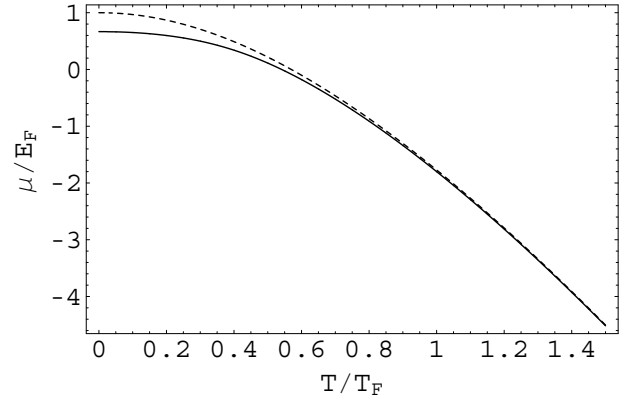


FIG. 4: The relationship between chemical potential and the rescaled temperature. The line styles are the same as in Fig.1.

From Eqs.(16) and (18), the entropy per particle as a function of the rescaled temperature is indicated in Fig.5. In Fig.6, the isochore heat capacity per particle related with the rescaled temperature is presented. The numerical results are obtained by solving the coupled Eqs.(16) and (22).

Near the Boltzmann regime, the energy, chemical potential, entropy and isochore heat capacity of a trapped unitary Fermi gas are getting closer to and almost overlap with those of the trapped ideal Fermi gas. In the low-temperature strong degenerate regime, the thermodynamic quantities of the unitary gas are lower than the ones of the ideal gas at the same temperature. The energy, chemical potential and entropy of a unitary gas are always lower than the ideal ones at the same temperature. However, as shown in Fig.6, the isochore heat capacity

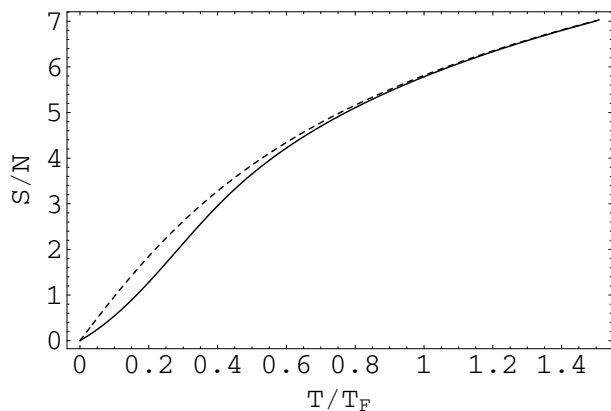


FIG. 5: Same as in Fig.4 for entropy per particle plotted as a function of the scaled temperature.

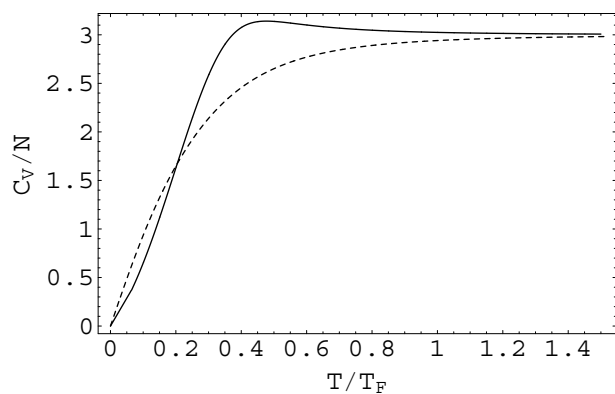


FIG. 6: Plot of the isochore heat capacity per particle as a function of the scaled temperature. The line styles are the same as those shown in Fig.5.

per particle given by the fractional exclusion statistics is

not a naive monotonously increasing function with the increase of the scaled temperature. This behavior is different from that of the trapped ideal Fermi gas.

IV. CONCLUSION

The finite-temperature thermodynamic quantities of a trapped unitary Fermi gas have been discussed in terms of the approved fractional exclusion statistics framework. The study shows that the thermodynamic quantities of a trapped unitary Fermi gas will overlap with those of the trapped ideal Fermi gas in the Boltzmann regime. The thermodynamic quantities given by this formalism are lower than the trapped ideal ones at the same temperature except for the isochore heat capacity.

The energy and entropy per particle manifest the consistency with the low-temperature experimental measurement. However, the detailed numerical study of the chemical potential shows that there is an explicit difference between the result given in terms of fractional exclusion statistics and experimental data in the weakly degenerate regime. For the three-dimensional trapped unitary Fermi gas, the high-temperature weakly degenerate behavior of chemical potential given by a simple fractional exclusion statistics hypothesis needs clarifying further.

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